

# Spectroscopic Studies of Some Diatomic Molecules using Spectrum Generating Algebra Approach

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## Abstract

For arbitrary values  $n$  and  $\ell$  quantum numbers, we present the solutions of the 3-dimensional Schrödinger wave equation with the pseudoharmonic potential via  $SU(1, 1)$  Spectrum Generating Algebra (SGA) approach. The explicit bound state energies and eigenfunctions are obtained. The matrix elements  $r^2$  and  $r \frac{d}{dr}$  are obtained (in a closed form) directly from the creation and annihilation operators. In addition, the expectation values of  $r^2$  and  $p^2$  and the Heisenberg Uncertainty Products (HUP) for set of diatomic molecules ( $O_2, I_2, N_2, H_2, CO, NO, HCl, CH, LiH, ScH, TiH, VH, CrH, MnH, TiC, NiC, ScN, ScF, Ar_2$ ) for arbitrary values of  $n$  and  $\ell$  quantum numbers are obtained. The results obtained are in excellent agreement with the available results in the literature. It is also shown that the HUP is obeyed for all diatomic molecules considered.

**KEY WORDS:** Schrödinger equation, explicit bound state energies, eigenfunctions, matrix elements, expectation values, ladder operators,  $SU(1, 1)$ , pseudoharmonic potential, diatomic molecules, Hellmann-Feynman theorem, Heisenberg Uncertainty Principle.

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## 1 Introduction

The Spectrum Generating Algebra (SGA) methods have been playing an important role in solving some quantum mechanical problems, since its introduction by Schrödinger, Infeld, Infeld and Hull [1, 2]. This technique serves as a useful tool in various fields of physics, ranging from quantum mechanics (relativistic and nonrelativistic), mathematical

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physics, optics, solid state physics, nuclear physics to chemical physics. This can be achieved through the construction of the ladder operators (creation and annihilation operators) or raising and lowering operators. From these ladder operators, the compact dynamical algebraic groups (a suitable Lie algebra) that such system belongs can be easily realized [3 - 23].

It should be noted that, Schrödinger factorization method has been less frequently applied to physical systems than Infeld-Hull factorization method, as it has been analyzed in detail by Martínez et al. [19], and exemplified later with a typical system [18]. Martínez and Mota presented a systematic procedure of using the factorization method to construct the generators for hidden and dynamical symmetries, and applied this study to  $2D$  problems of hydrogen atom, the isotropic harmonic and other radial potential of interest.

This algebraic approach has been successfully applied to a set of model potentials such as the with Morse potential, Pöschl-Teller potential, pseudoharmonic potential, infinite square well in  $3D$  as well as  $N$ -dimensions [4, 7 - 23] and their energy spectrum and the eigenfunctions have been studied.

The  $SU(1, 1)$  dynamical algebra from the Schrödinger ladder operators for hydrogen atom, Mie-type potential, harmonic oscillator and pseudoharmonic oscillator for  $N$ -dimensional systems have been extensively discussed by Martínez et al. [19]. In the similar fashion, Salazar-Ramírez et al. [20, 21] have applied the factorization method to construct the generators of the dynamical algebra  $SU(1, 1)$  for the radial equation of the non-relativistic and relativistic generalized MICZ-Kepler problem. It should be noted that the generators in the examples[18, 19, 20, 21] above have been constructed without adding phase as an additional variable like in Martínez-y-Romero et al. [8].

Gur and Mann [16] have used the  $SU(1, 1)$  SGA method to construct the associated radial Barut-Girardello coherent states for the isotropic harmonic oscillator in arbitrary dimension and these states have been mapped into the Sturm-Coulomb radial coherent states. The dynamics of the  $SU(1, 1)$  coherent states for the time-dependent quadratic hamiltonian system has been discussed by Choi [22].

In their work, Motavalli and Akbarieh [23] presented a general construction for the

ladder operators for special orthogonal functions based on the Nikiforov-Uvarov formalism and generated a list of creation and annihilation operators for some well known special functions.

In the present study, we have followed the approach introduced by Dong [4]. This is done by using the recursion relations for the generalized Laguerre polynomials and the explicit form of the eigenfunctions, the  $SU(1, 1)$  dynamical algebra generators for some quantum mechanical systems can therefore be obtained.

Apart from generating the eigenvalues and eigenfunctions, this approach offers the additional advantages in that it can be used to find the matrix elements in a simple way, and it is also very useful in constructing coherent states of a given Hamiltonian system [16, 22, 24]. Thus, Gur and Mann [16] used SGA approach to construct the radial Barut-Girardello coherent states for the isotropic harmonic oscillator in arbitrary dimension and mapped these states into Sturm-Coulomb radial coherent state; the dynamics of  $SU(1, 1)$  coherent states are investigated for the time-dependent quadratic Hamiltonian system by Choi [22]. Very recently, the second lowest and second highest bases of the discrete positive and negative irreducible representations of  $SU(1, 1)$  Lie algebra via spherical harmonics are used to construct generalized coherent states by Dehghani and Fakhri [24].

In recent years, discussion on the 3D-dimensional anharmonic oscillators has been receiving considerable attention in chemical physics. This is due to their usefulness in studying the dynamical variables of diatomic molecules. The Morse potential has been one of the most popular model potential which is employed in the study of molecular spectra [36 - 38, 41 - 44].

The corresponding wavefunction does not vanish at the origin, and the exact solutions for any angular momentum ( $\ell \neq 0$ ) are as yet unknown. Several other potentials are been used as alternatives and their performances have been compared with the Morse potential [39, 40, 42]. For examples, Kratzer and pseudoharmonic potentials which have known exact solutions like in the Coulomb and harmonic oscillator model potentials [17, 35, 44, 45, 46, 47, 48].

For the purpose of this study, we consider pseudoharmonic potential. This potential

has been very useful in the area of physical sciences and it has been extensively used to describe interaction of some diatomic molecules since its introduction [4, 15, 25, 26, 27, 29, 33, 34, 35]. Sage [26] has discussed the energy levels and wavefunctions of a rotating diatomic molecule using a three-parameter model potential called the pseudogaussian (pseudoharmonic) potential and he found that the potential is reasonably behaved for both small and large internuclear separations.

Obviously, the pseudoharmonic oscillator behaves asymptotically as a harmonic oscillator, but has a minimum at  $r = r_e$  and exhibits a repulsive inverse-square-type singularity at  $r = 0$ . The energy eigenvalues and the eigenfunctions of the pseudoharmonic oscillator can be found exactly for any angular momentum. These wavefunctions have reasonable behaviour at the origin, near the equilibrium, and at the infinity [28].

Its characteristics make it useful to model various physical systems, including some molecular physical ones [4, 17, 26, 27, 34, 46]. From the mathematical point of view, it resembles the harmonic oscillator, from which it deviates by two correction terms depending on the potential depth and the equilibrium distance parameter  $r_e$ : the first one is an energy shift and the second one is a modified centrifugal term. The latter can also be viewed as originating formally from a non-integer orbital angular momentum [27]. The eigenfunctions and energy eigenvalues are similar to those of the harmonic oscillator, which can be obtained exactly in the  $r_e \rightarrow 0$  limit.

Recently, with an improved approximation to the orbital centrifugal term of the Manning-Rosen potential, Ikhdaïr [49] used the nikiforov-Uvarov method to obtain the rotational-vibrational energy states for a few diatomic molecules for arbitrary quantum numbers  $n$  and  $\ell$  with different values of the potential parameters.

In the study of the diatomic molecules using the diatomic molecular potentials, different methods have been employed: Nikiforov-Uvarov method [35, 41 - 46]; asymptotic iteration method [47]; Exact method [34]; shifted  $1/N$  expansion [37]; exact quantization rule method [39, 48]; SUSY approach [38]; Nikiforov-Uvarov method [35, 44, 46]; tridiagonal J-matrix representation [51] and algebraic method [17, 50].

The aim of this work is to realize the dynamical  $SU(1,1)$  algebra generators for the pseudoharmonic potential to obtain the energy eigenvalues, eigenfunctions and the

matrix elements of the pseudoharmonic potential. The results obtained are used to calculate the bound state energies of some neutral diatomic molecules (metallic hydrides, homogeneous and heterogeneous diatomic molecules) for any  $n$  and  $\ell$  quantum numbers.

The scheme of our presentation is as follows: in Section 2, we study the 3-dimensional Schrödinger equation for the pseudoharmonic potential. In Section 3, we present the formal solutions of the problem and describe the SGA method used in constructing the ladder operators for obtaining the energy eigenvalues, the eigenfunctions and the matrix elements for the pseudoharmonic potential. We present in Section 4, the explicit bound state energies, the numerical values of the expectation values of  $r^2$  and  $p^2$  and the Heisenberg uncertainty product for the pseudoharmonic potential for the homogeneous diatomic molecules ( $O_2, I_2, N_2, H_2, Ar_2$ ); the heterogeneous diatomic molecules (CO, NO, HCl, CH, LiH); the neutral transition metal hydrides (ScH, TiH, VH, CrH, MnH); the transition-metal lithide (CuLi); the transition-metal carbides (TiC, NiC); the transition-metal nitride (ScN) and the transition-metal fluoride (ScF). Finally, in Section 5, we discuss our conclusions.

## 2 The 3-dimensional Schrödinger equation for the pseudoharmonic potential

The pseudoharmonic-type potential can be written in the standard form as [4, 15, 31, 32, 33, 34]

$$V(r) = Ar^2 + \frac{B}{r^2} + c. \quad (1)$$

This potential is associated with the following molecular potentials:

- Isotropic harmonic oscillator plus inverse quadratic potential

$$V(r) = \mu\omega^2 \frac{r^2}{2} + \frac{g}{r^2}, \quad (2)$$

here  $A = \mu\omega^2$ ,  $B = g$  and  $c = 0$  [4, 15, 29, 31, 32, 33].

- The pseudoharmonic potential

$$V(r) = D_e \left( \frac{r}{r_e} - \frac{r_e}{r} \right)^2, \quad (3)$$

where  $D_e$  is the dissociation energy between two atoms in a solid and  $r_e$  is the equilibrium intermolecular separation. Here, we have  $A = \frac{D_e}{r_e^2}$ ,  $B = D_e r_e$  and  $c = -2D_e$  [4, 15, 25 - 32, 35]. The graphs of the potential in equation(3) for some diatomic molecules is displayed in the figure below **Figure 1**.

**Figure 1.** Shapes of the pseudoharmonic potentials for some diatomic molecules.

The Schrödinger equation for the three-dimension for this potential is

$$\left[ -\frac{\hbar^2}{2\mu} \Delta + \frac{D_e}{r_e^2} r^2 + \frac{D_e r_e^2}{r^2} - 2D_e \right] \psi(r, \theta, \phi) = E \psi(r, \theta, \phi). \quad (4)$$

If we propose  $\psi_{n,\ell,m}(r, \theta, \phi)$  to have the form

$$\psi_{n,\ell,m}(r, \theta, \phi) = R_{n,\ell,m}(r) Y_{\ell,m}(\theta, \phi) \quad (5)$$

then, equation (4) reduces to two decoupled differential equations, that is, the radial and angular wavefunctions:

$$\left\{ \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} + \left[ \frac{2\mu}{\hbar^2} \left[ E - \left( \frac{D_e}{r_e^2} r^2 + \frac{D_e r_e^2}{r^2} - 2D_e \right) \right] - \frac{\ell(\ell+1)}{r^2} \right] \right\} R_{n,\ell}(r) = 0 \quad (6)$$

and

$$L^2 Y_{\ell,m}(\theta, \phi) = \hbar^2 \ell(\ell+1) Y_{\ell,m}(\theta, \phi), \quad (7)$$

where  $\ell = 0, 1, 2, \dots$  is the orbital angular momentum quantum numbers,  $n = 1, 2, 3, \dots$  is the principal quantum number,  $\mu$  is the reduced mass,  $\hbar$  is the Planck's constant divided by  $2\pi$  and  $E$  is the energy eigenvalue. Equation (6) can be rewritten as

$$\left\{ \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} + \left[ K^2 + \frac{4\mu D_e}{\hbar^2} - \frac{2\mu D_e}{\hbar^2 r_e^2} r^2 - \frac{\gamma_\ell(\gamma_\ell+1)}{r^2} \right] \right\} R_{n,\ell}(r) = 0, \quad (8)$$

where

$$\gamma_\ell = \frac{1}{2} \left[ -1 + \sqrt{(2\ell+1)^2 + \frac{8\mu D_e r_e^2}{\hbar^2}} \right]. \quad (9)$$

To obtain the relevant algebraic operators for the radial symmetry, equation (8) is solved and the solutions which is a degenerate hypergeometric or Kummer equation (associated Laguerre differential equation) is obtained [52 - 54]. Then, the radial funtions  $R_{n,\ell}(r)$  for this potential is obtained as:

$$R_{n,\ell}(r) = N_{n,\ell} r^{\gamma_\ell} e^{-\lambda r^2} L_n^{\gamma_\ell + \frac{1}{2}}(2\lambda r^2), \quad (10)$$

where

$$\lambda = \sqrt{\frac{\mu D_e}{2\hbar^2 r_e^2}}. \quad (11)$$

$L_n^k(x)$  is the associated Laguerre functions [52 - 54],  $N_{n,\ell}$  is the normalization constant which is determined from the normalization condition

$$\int_0^\infty R_{n,\ell}(r) R_{n',\ell}(r) dr = \delta_{n,n'} \quad (12)$$

as

$$N_{n,\ell} = \left[ \frac{2(2\lambda^2)^{\frac{1}{4}(2\gamma_\ell+3)} n!}{\Gamma(n + \gamma_\ell + \frac{3}{2})} \right]^{\frac{1}{2}}. \quad (13)$$

### 3 The Spectrum Generating Algebra (SGA)

In a brief introduction, the classical Lie algebra  $SU(1,1)$  can be generated by the elements  $K_0, K_1, K_2$  which satisfies the following commutation relations:

$$[K_0, K_1] = iK_2, \quad [K_1, K_2] = -iK_0, \quad [K_2, K_0] = iK_1. \quad (14)$$

Alternatively, these can be expressed in terms of the creation and annihilation operators

$$K_\pm = K_1 \pm iK_2, \quad (15)$$

the commutation relations together with  $K_0$  can be written as:

$$[K_0, K_\pm] = \pm K_\pm, \quad [K_-, K_+] = 2K_0. \quad (16)$$

Based on the Schrödinger factorization method, Infeld-Hull factorization method, we adopt the factorization method introduced by Dong [4]. This is done by construction of the creation and annihilation operators through the recursion relations of the Laguerre functions that evolved, and thereby construct a suitable Lie algebra in terms of these ladder operators.

In this case, we obtain the differential operators  $\hat{\mathcal{J}}_\pm$  with the following property:

$$\hat{\mathcal{J}}_\pm R_{n,\ell}(r) = j_\pm R_{n_r \pm 1, \ell}(r), \quad (17)$$

these operators are of the form

$$\hat{\mathcal{J}}_{\pm} = A_{\pm}(r) \frac{d}{dr} + B_{\pm}(r) \quad (18)$$

and depend only on the physical variable  $r$ .

On operating the differential operator  $\frac{d}{dr}$  on the radial wavefunctions (10), we have,

$$\frac{d}{dr} R_{n,\ell}(r) = \frac{\gamma_{\ell}}{r} R_{n,\ell}(r) - 2\lambda r R_{n,\ell}(r) + N_{n,\ell} r^{\gamma_{\ell}} \exp(-\lambda r^2) \frac{d}{dr} L_n^{\gamma_{\ell} + \frac{1}{2}}(2\lambda r^2). \quad (19)$$

In order to find the relationship between  $R_{n,\ell}(r)$  and  $R_{n+1,\ell}(r)$ , the expression above is used to construct the ladder operators  $\hat{\mathcal{J}}_{\pm}$  by using the recurrence relations of the associated Laguerre functions. To find these, the following recurrence relations of the associated Laguerre functions are used [52 - 54]:

$$x \frac{d}{dx} L_n^{\alpha}(x) = \begin{cases} n L_n^{\alpha}(x) - (n + \alpha) L_{n-1}^{\alpha}(x) \\ (n + 1) L_{n+1}^{\alpha}(x) - (n + \alpha + 1 - x) L_n^{\alpha}(x) \end{cases} \quad (20)$$

The creation and annihilation operators are obtained as:

$$\hat{\mathcal{J}}_- = \frac{1}{2} \left[ -r \frac{d}{dr} - 2\lambda r^2 + 2\hat{n} + \gamma_{\ell} \right]; \quad \hat{\mathcal{J}}_+ = \frac{1}{2} \left[ r \frac{d}{dr} - 2\lambda r^2 + 2\hat{n} + \gamma_{\ell} + 3 \right], \quad (21)$$

where  $\hat{n}$  is the number operator with the property

$$\hat{n} R_{n,\ell}(r) = n R_{n,\ell}(r). \quad (22)$$

On defining the operator

$$\hat{\mathcal{J}}_0 = \frac{1}{4} \left[ -\frac{d^2}{dr^2} - \frac{2}{r} \frac{d}{dr} + \frac{\gamma_{\ell}(\gamma_{\ell} + 1)}{r^2} + \frac{2\mu D_e r^2}{\hbar^2 r_e^2} \right], \quad (23)$$

then, the operation of  $\hat{\mathcal{J}}_{\pm}$  and  $\hat{\mathcal{J}}_0$  on the radial wavefunctions  $R_{n,\ell}(r)$  allows us to find the following properties:

$$\hat{\mathcal{J}}_+ R_{n,\ell}(r) = \sqrt{(n+1) \left( n + \gamma_{\ell} + \frac{3}{2} \right)} R_{n+1,\ell}(r) = j_+ R_{n+1,\ell}(r), \quad (24)$$

$$\hat{\mathcal{J}}_- R_{n,\ell}(r) = \sqrt{n \left( n + \gamma_{\ell} + \frac{1}{2} \right)} R_{n-1,\ell}(r) = j_- R_{n-1,\ell}(r), \quad (25)$$

$$\hat{\mathcal{J}}_0 R_{n,\ell}(r) = n + \frac{2\gamma_{\ell} + 3}{4} R_{n,\ell}(r) = j_0 R_{n,\ell}(r). \quad (26)$$



On carefully inspecting the dynamical group associated to the annihilation and creation operators  $\hat{\mathcal{J}}_-$  and  $\hat{\mathcal{J}}_+$ , based on the results of equations (24) and (25), the commutator  $[\hat{\mathcal{J}}_-, \hat{\mathcal{J}}_+]$  can be evaluated as follows:

$$[\hat{\mathcal{J}}_-, \hat{\mathcal{J}}_+]R_{n,\ell}(r) = 2j_0 R_{n,\ell}(r), \quad (27)$$

where  $j_0 = n + \frac{2\gamma_\ell+3}{4}$  and operators  $\hat{\mathcal{J}}_\mp$  and  $\hat{\mathcal{J}}_0$  satisfy the following commutation relations:

$$[\hat{\mathcal{J}}_0, \hat{\mathcal{J}}_\mp]R_{n,\ell}(r) = \mp \hat{\mathcal{J}}_\mp R_{n,\ell}(r). \quad (28)$$

We define the Hermitian operators for these operators as follows:

$$\hat{\mathcal{J}}_x = \frac{1}{2}(\hat{\mathcal{J}}_+ + \hat{\mathcal{J}}_-), \quad \hat{\mathcal{J}}_y = \frac{1}{2i}(\hat{\mathcal{J}}_+ - \hat{\mathcal{J}}_-), \quad \hat{\mathcal{J}}_z = \hat{\mathcal{J}}_0 \quad (29)$$

and the following commutation relations are obtained:

$$[\hat{\mathcal{J}}_x, \hat{\mathcal{J}}_y] = -i\hat{\mathcal{J}}_z, \quad [\hat{\mathcal{J}}_y, \hat{\mathcal{J}}_z] = i\hat{\mathcal{J}}_x, \quad [\hat{\mathcal{J}}_z, \hat{\mathcal{J}}_x] = i\hat{\mathcal{J}}_y. \quad (30)$$

The Casimir operator can be expressed as [55]

$$\begin{aligned} \hat{\mathcal{C}}R_{n,\ell}(r) &= \{\hat{\mathcal{J}}_0(\hat{\mathcal{J}}_0 - 1) - \hat{\mathcal{J}}_+\hat{\mathcal{J}}_-\} R_{n,\ell}(r) = \{\hat{\mathcal{J}}_0(\hat{\mathcal{J}}_0 + 1) - \hat{\mathcal{J}}_-\hat{\mathcal{J}}_+\} R_{n,\ell}(r) \\ &= \left(\frac{2\gamma_\ell+3}{4}\right) \left(\frac{2\gamma_\ell-1}{4}\right) R_{n,\ell}(r) = \tau(\tau - 1)R_{n,\ell}(r), \end{aligned} \quad (31)$$

where

$$\tau = \frac{2\gamma_\ell + 3}{4}. \quad (32)$$

Then, the Casimir operator  $\hat{\mathcal{C}}$  now satisfies the following commutation relations:

$$[\hat{\mathcal{C}}, \hat{\mathcal{J}}_\pm] = [\hat{\mathcal{C}}, \hat{\mathcal{J}}_x] = [\hat{\mathcal{C}}, \hat{\mathcal{J}}_y] = [\hat{\mathcal{C}}, \hat{\mathcal{J}}_z] = 0, \quad (33)$$

therefore, the operators  $\hat{\mathcal{J}}_\pm$ ,  $\hat{\mathcal{J}}_x$ ,  $\hat{\mathcal{J}}_y$ ,  $\hat{\mathcal{J}}_z$  and  $\hat{\mathcal{J}}_0$  satisfy the commutation relations of the dynamical group  $SU(1, 1)$  algebra, which is isomorphic to an  $SO(2, 1)$  algebra (i. e.  $SU(1, 1) \sim SO(2, 1)$ ). The commutation rules are valid for the infinitesimal operators of the non-compact group  $SU(1, 1)$  [9, 56].

The Hamiltonian operator  $\hat{\mathcal{H}}$  takes the form

$$\hat{\mathcal{H}} = (4n + 2\gamma_\ell + 3) \sqrt{\frac{\hbar^2 D_e}{2\mu r_e^2}} - 2D_e = \frac{1}{4}\hat{\mathcal{J}}_0 \sqrt{\frac{\hbar^2 D_e}{2\mu r_e^2}} - 2D_e. \quad (34)$$

Furthermore, we find that the following physical functions can be obtained by the creation and annihilation operators  $\hat{\mathcal{J}}_{\mp}$  and  $\hat{\mathcal{J}}_0$  as:

$$r^2 R_{n,\ell}(r) = \frac{1}{2\lambda} [2\hat{\mathcal{J}}_0 - (\hat{\mathcal{J}}_+ + \hat{\mathcal{J}}_-)] R_{n,\ell}(r), \quad (35)$$

$$r \frac{d}{dr} R_{n,\ell}(r) = (\hat{\mathcal{J}}_+ - \hat{\mathcal{J}}_-) - \frac{3}{2} R_{n,\ell}(r). \quad (36)$$

With equations (35) and (36), the matrix elements for  $r^2$  and  $r \frac{d}{dr}$  are obtained as follows:

$$\begin{aligned} & \langle R_{m,\ell}(r) | r^2 | R_{n,\ell}(r) \rangle \\ &= \frac{1}{2\lambda} \left[ \left( 2n + \frac{2\gamma_\ell + 3}{2} \right) \delta_{m,n} - j_+ \delta_{m,n+1} - j_- \delta_{m,n-1} \right] \end{aligned} \quad (37)$$

and

$$\begin{aligned} & \langle R_{m,\ell}(r) | r \frac{d}{dr} | R_{n,\ell}(r) \rangle \\ &= j_+ \delta_{m,n+1} - j_- \delta_{m,n-1} - \frac{3}{2} \delta_{m,n}. \end{aligned} \quad (38)$$

From the relations above, we can deduce the following relations:

$$2\lambda \langle R_{m,\ell}(r) | r^2 | R_{n,\ell}(r) \rangle + \langle R_{m,\ell}(r) | r \frac{d}{dr} | R_{n,\ell}(r) \rangle = (2n + \gamma_\ell) \delta_{m,n} - 2j_- \delta_{m,n-1} \quad (39)$$

and

$$2\lambda \langle R_{m,\ell}(r) | r^2 | R_{n,\ell}(r) \rangle - \langle R_{m,\ell}(r) | r \frac{d}{dr} | R_{n,\ell}(r) \rangle = (2n + \gamma_\ell + 3) \delta_{m,n} - 2j_+ \delta_{m,n+1}. \quad (40)$$

These two relations form a useful link for finding the matrix elements from the creation and annihilator operators.

## 4 The explicit bound state energies, the numerical values of $\langle r^2 \rangle$ , $\langle p^2 \rangle$ and the Heisenberg Uncertainty Products

### 4.1 The explicit bound state energies for the pseudoharmonic potential

The explicit bound state energies for the pseudoharmonic potential are obtained as :

$$E_{n,\ell} = (4n + 2\gamma_\ell + 3) \sqrt{\frac{\hbar^2 D_e}{2\mu r_e^2}} - 2D_e, \quad (41)$$

where  $\gamma_\ell$  is as stated in equation (9).

## 4.2 The expectation values of $r^2$ and $p^2$ for the pseudoharmonic potential

The expectation values of  $r^2$  and  $p^2$  can be obtained by applying the Hellmann-Feynman theorem (HFT) [30, 57 - 64]. This theorem states that a non-degenerate eigenvalue of a hermitian operator in a parameter dependent eigensystem varies with respect to the parameter according to the formula

$$\frac{\partial E_\nu}{\partial \nu} = \langle \Psi_\nu | \frac{\partial H_\nu}{\partial \nu} | \Psi_\nu \rangle, \quad (42)$$

provided that the associated normalized eigenfunction  $\Psi_\nu$ , is continuous with respect to the parameter,  $\nu$ . The effective Hamiltonian of the pseudoharmonic potential radial wave function is

$$\hat{\mathcal{H}} = \frac{-\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2} + \frac{D_e}{r_e^2} r^2 + \frac{D_e r_e^2}{r^2} - 2D_e. \quad (43)$$

With  $\nu = D_e$  and  $\nu = \mu$ , then, the following expectation values of  $r^2$  and  $p^2$  are obtained respectively as:

$$\langle r^2 \rangle = \left[ 2n + 1 + \frac{1}{2} \sqrt{(2\ell + 1)^2 + \frac{8\mu D_e r_e^2}{\hbar^2}} \right] \sqrt{\frac{\hbar^2 r_e^2}{2\mu D_e}} \quad (44)$$

and

$$\begin{aligned} \langle p^2 \rangle = 2\mu D_e & \left[ 2n + 1 + \frac{1}{2} \sqrt{(2\ell + 1)^2 + \frac{8\mu D_e r_e^2}{\hbar^2}} \right] \sqrt{\frac{\hbar^2}{2\mu D_e r_e^2}} \\ & - \frac{4\mu D_e}{\sqrt{(2\ell + 1)^2 + \frac{8\mu D_e r_e^2}{\hbar^2}}} \sqrt{\frac{2\mu D_e r_e^2}{\hbar^2}}. \end{aligned} \quad (45)$$

## 4.3 The Heisenberg Uncertainty product for the pseudoharmonic potential

In 1927, Werner Heisenberg stated that certain physical quantities, like the position and momentum, cannot both have precise values at the same time, this is called the Heisenberg uncertainty principle [65]. That is, the more precisely one property is measured, the less precisely the other can be measured. A mathematical statement of this principle is

that every quantum state has the property that the root mean square (RMS) deviation of the position from its mean (the standard deviation of the x-distribution):

$$\Delta x = \sqrt{\langle (x - \langle x \rangle)^2 \rangle} \quad (46)$$

and the RMS deviation of the momentum from its mean (the standard deviation of p):

$$\Delta p_x = \sqrt{\langle (p_x - \langle p_x \rangle)^2 \rangle}, \quad (47)$$

the product of which can never be smaller than a fixed fraction of Planck's constant:

$$\Delta x \Delta p_x \geq \frac{\hbar}{2}. \quad (48)$$

This inequality is very important in physics, it has been pointed out that for a particle moving non-relativistically in a central potential  $V(r)$ , the following uncertainty relation holds [33, 61, 62, 64, 65, 66]:

$$\Delta r \Delta p \geq \frac{3\hbar}{2}. \quad (49)$$

With equations (44) and (46) and noting that  $\langle r \rangle = \langle p \rangle = 0$  (due to parity consideration), the Heisenberg uncertainty product for the pseudoharmonic potential becomes:

$$P_{n,\ell} = \Delta r \Delta p = \left[ 2n + 1 + \frac{1}{2} \sqrt{(2\ell + 1)^2 + \frac{8\mu D_e r_e^2}{\hbar^2}} \right]^2 \hbar^2 \quad (50)$$

$$- \frac{4\mu D_e r_e^2}{\sqrt{(2\ell + 1)^2 + \frac{8\mu D_e r_e^2}{\hbar^2}}} \left[ 2n + 1 + \frac{1}{2} \sqrt{(2\ell + 1)^2 + \frac{8\mu D_e r_e^2}{\hbar^2}} \right].$$

In this work, we obtained the explicit bound state energies ( $E_{n,\ell}$ ), the expectation values of  $r^2$  and  $p^2$  ( $\langle r^2 \rangle$  and  $\langle p^2 \rangle$ ) and the Heisenberg uncertainty product  $P_{n,\ell}$  of some diatomic molecules for various values of  $n$  and  $\ell$ . In the case of this study, we have selected some diatomic molecules for the purposes which they serve in various aspect of chemical synthesis, nature of bonding, temperature stability and electronic transport properties in chemical physics [41, 70, 72].

Some of these selected diatomic molecules composed of the some homogeneous diatomic molecules (dimers) ( $O_2, I_2, N_2, H_2, Ar_2$ ); the heterogeneous diatomic molecules (CO, NO, HCl, CH, LiH); the neutral transition metal hydrides ( ScH, TiH, VH, CrH,

MnH); the transition-metal lithide (CuLi); the transition-metal carbides (TiC, NiC); the transition-metal nitride (ScN) and the transition-metal fluoride(ScF).

The spectroscopic parameters and reduced masses for some selected diatomic molecules used in our study are shown in Table 1. The spectroscopic parameters listed in this table are obtained from the following cited sources: for CO, NO,  $O_2$ ,  $I_2$  and  $N_2$ , the sources are [34, 35, 45, 47, 48, 68, 69]; for CH, LiH and HCl, the sources are [34, 35, 39, 43, 45, 48, 68, 73] ; for  $H_2$ , the source is [74] ; for  $Ar_2$ , the source is [71, 72] and for ScH, TiH, VH, CrH, MnH, CuLi, TiC, NiC, ScN and ScF, the sources are [41, 70], where  $\hbar c = 1973.29 \text{ eV}\text{\AA}^\circ$  is taken from [34, 35, 41, 43, 45, 47, 48, 49, 76].

For these selected diatomic molecules, we have available results from the literature to compare with our results with few ones: CO, NO, CH and  $N_2$  [34, 35].

The explicit bound state energies of some of these diatomic molecules for various values of  $n$  and  $\ell$  are obtained and compared with the exact method [34] and the Nikiforov-Uvarov method [35] for CO, NO, CH and  $N_2$ . In the Tables 2 - 7, we have used  $E_{n,\ell}$  (FM) to mean factorization method (present method),  $E_{n,\ell}$ (EM) to mean Exact Method [34] and  $E_{n,\ell}$  (NU) mean Nikiforov-Uvarov Method [35]. Also, the numerical results for the expectation values of  $r^2$  and  $p^2$  ( $\langle r^2 \rangle$  and  $\langle p^2 \rangle$ ) and the Heisenberg uncertainty product  $P_{n,\ell}$  of some of these diatomic molecules for various values of  $n$  and  $\ell$  are computed and

Table 1: Model parameters for some diatomic molecules in our study.

Molecules	$D_e$ (in eV)	$r_e$ (in $\text{\AA}^\circ$ )	$\mu$ (in amu)	Molecules	$D_e$ (in eV)	$r_e$ (in $\text{\AA}^\circ$ )	$\mu$ (in amu)
<i>ScH</i>	2.25	1.776	0.986040	<i>CH</i>	3.947418665	1.1198	0.929931
<i>TiH</i>	2.05	1.781	0.987371	<i>LiH</i>	2.5152672118	1.5956	0.8801221
<i>VH</i>	2.33	1.719	0.988005	<i>HCl</i>	4.619030905	1.2746	0.9801045
<i>CrH</i>	2.13	1.694	0.988976	$H_2$	4.7446	0.7416	0.50391
<i>MnH</i>	1.67	1.753	0.989984	<i>CO</i>	10.845073641	1.1282	6.860586000
<i>CuLi</i>	1.74	2.310	6.259494	<i>NO</i>	8.043729855	1.1508	7.468441000
<i>TiC</i>	2.66	1.790	9.606079	$O_2$	5.156658828	1.208	7.997457504
<i>NiC</i>	2.76	1.621	9.974265	$I_2$	1.581791863	2.662	63.45223502
<i>ScN</i>	4.56	1.768	10.682771	$N_2$	11.938193820	1.0940	7.00335
<i>ScF</i>	5.85	1.794	13.358942	$Ar_2$	1.672	2.53	53.9341

presented in Tables 2 - 7.

Table 2: The energy eigenvalues  $E_{n,\ell}$  (in eV), the expectation values  $\langle r^2 \rangle$  (in  $(A^o)^2$ ),  $\langle p^2 \rangle$  (in  $(eV/c)^2$ ) and the Heisenberg Uncertainty Relations HUR (in  $eVA^o/c$ ) corresponding to the pseudoharmonic potential for various  $n$  and  $\ell$  quantum numbers for  $CO$  and  $NO$  diatomic molecules.

$n$	$\ell$	$E_{n,\ell}$ [FM]	$E_{n,\ell}$ [EM]	$E_{n,\ell}$ [NU]	$\langle r^2 \rangle$	$\langle p^2 \rangle$	HUR
<b>CO</b>							
0	0	0.1019578053531127	0.1019306	0.10193061	1.278818514996878	651953274.6811209	28874.38170030767
1	0	0.3057536875651401	0.3056722	0.30567217	1.290777797622587	1954330222.150913	50225.55186332170
	1	0.3062325780354271	0.3061508	0.30615078	1.290805888935957	1960448477.813082	50304.65624687896
2	0	0.5095495697771710	0.5094137	0.50941373	1.302737080248297	3256707169.620706	65135.49868831414
	1	0.5100284602474545	0.5098923	0.50989234	1.302765171561666	3262825425.282874	65197.35673280329
	2	0.5109862411880286	0.5108495	0.51084953	1.302821352328619	3275061126.516209	65320.89685396806
4	0	0.9171413342012258	0.9168969	0.91689685	1.326655645499716	5861461064.560290	88182.42688980432
	1	0.9176202246715128	0.9173755	0.91737546	1.326683736813085	5867579320.222428	88229.37185880831
	2	0.9185780056120834	0.9183327	0.91833265	1.326739917580037	5879815021.455794	88323.18663268512
	3	0.9200131221837502	0.9197684	0.91976835	1.326824184081614	5898166548.480750	88463.72148098587
	4	0.9219286840648948	0.9216825	0.92168247	1.326936530740917	5922631472.632870	88650.75329151144
5	0	1.120937216413253	1.1206384	1.12063840	1.338614928125425	7163838012.030083	97926.60775078365
	1	1.121416106883540	1.1211170	1.12111700	1.338643019438795	7169956267.692221	97969.44374358583
	2	1.122373887824111	1.1220742	1.12207420	1.338699200205747	7182191968.925556	98055.05925001923
	3	1.123809004395778	1.1235099	1.12350990	1.338783466707324	7200543495.950542	98183.34168119120
	4	1.125724566276922	1.1254240	1.12542400	1.338895813366626	7225008420.102662	98354.12307175575
	5	1.128117463789163	1.1278165	1.12781650	1.339036232750661	7255583505.037642	98567.18116591059
<b>NO</b>							
0	0	0.08251086588683876	0.0824883	0.08248827	1.331132968244588	574375573.8664465	27650.86368502856
1	0	0.2474257254889523	0.2473592	0.24735916	1.344708974060483	1721656608.599298	48115.76760100594
	1	0.2478484808663488	0.2477817	0.24778171	1.344743765885460	1727536886.807932	48198.49021361709
2	0	0.4123405850910657	0.4122301	0.41223005	1.358284979876379	2868937643.332150	62424.63383264652
	1	0.4127633404684623	0.4126526	0.41265260	1.358319771701355	2874817921.540784	62489.37527988453
	2	0.4136075930227321	0.4134977	0.41349768	1.358389352609480	2886577551.185603	62618.65705212839
4	0	0.7421703042952892	0.7419718	0.74197183	1.385436991508170	5163499712.797879	84579.56909178477
	1	0.7425930596726857	0.7423944	0.74239438	1.385471783333147	5169379991.006488	84628.77829005003
	2	0.7434373122269555	0.7432395	0.74323946	1.385541364241271	5181139620.651306	84727.11052739678
	3	0.7447055783591487	0.7445070	0.74450700	1.385645728749967	5198776748.734846	84874.39423412152
	4	0.7463953416682116	0.7461969	0.74619689	1.385784868638066	5222288597.129426	85070.37391220915
5	0	0.9070851638974027	0.9068427	0.90684272	1.399012997324066	6310780747.530731	93962.03642460064
	1	0.9075079192747992	0.9072653	0.90726527	1.399047789149042	6316661025.739365	94006.97124609737
	2	0.9083521718290690	0.9081104	0.90811035	1.399117370057167	6328420655.384158	94096.77605516852
	3	0.9096204379612622	0.9093779	0.90937789	1.399221734565862	6346057783.467698	94231.32164752261
	4	0.9113102012703251	0.9110678	0.91106778	1.399360874453962	6369569631.862278	94410.41536789360
	5	0.9134227199567881	0.9131799	0.91317990	1.399534778764948	6398952498.950474	94633.80247007970

## 5 Conclusions

We have used  $SU(1, 1)$  spectrum generating algebra approach to obtain the solutions of the 3-dimensional Schrödinger wave equation with pseudoharmonic molecular potential. The explicit bound state energies, the eigenfunctions and the radial matrix elements are obtained for this molecular potential. Furthermore, based upon the solutions obtained,

Table 3: The energy eigenvalues  $E_{n,\ell}$ (in eV), the expectation values  $\langle r^2 \rangle$  (in  $(A^o)^2$ ),  $\langle p^2 \rangle$  (in  $(eV/c)^2$ ) and the Heisenberg Uncertainty Relations HUR (in  $eVA^o/c$ ) corresponding to the pseudoharmonic potential for various  $n$  and  $\ell$  quantum numbers for  $N_2$  and  $CH$  diatomic molecules.

$n$	$\ell$	$E_{n,\ell}$ [FM]	$E_{n,\ell}$ [EM]	$E_{n,\ell}$ [NU]	$\langle r^2 \rangle$	$\langle p^2 \rangle$	HUR
<b><math>N_2</math></b>							
0	0	0.1091860343455160	0.1091559	0.10915590	1.202309005240784	712683651.7236753	29272.27309853578
1	0	0.3274313753502547	0.3273430	0.32734304	1.213248845205456	2136424222.911053	50911.82791175150
	1	0.3279292342137836	0.3278417	0.32784167	1.213273844148512	2142930999.051733	50989.82379813161
2	0	0.5456767163549969	0.5455302	0.54553018	1.224188685170128	3560164794.098396	66017.52387265288
	1	0.5461745752185259	0.5460288	0.54602881	1.224213684113184	3566671570.239111	66078.49985452284
	2	0.5471719580253911	0.5470260	0.54702603	1.224263680432900	3579684307.137500	66200.28311604151
4	0	0.9821673983644743	0.9819045	0.98190446	1.246068365099471	6407645936.473118	89355.27346607656
	1	0.9826652572280032	0.9824031	0.98240309	1.246093364042527	6414152712.613832	89401.52756605153
	2	0.9836626400348720	0.9834003	0.98340031	1.246143360362243	6427165449.512221	89493.96376772718
	3	0.9851595467850807	0.9848961	0.98489606	1.246218350926318	6446682516.785655	89632.43863141369
	4	0.9871526473190038	0.9868903	0.98689026	1.246318331037525	6472701469.817430	89816.73837969733
5	0	1.200412739369217	1.2000916	1.20009160	1.257008205064143	7831386507.660496	99217.52414345898
	1	1.200910598232742	1.2005902	1.20059020	1.257033204007199	7837893283.801210	99259.72046708141
	2	1.201907981039611	1.2015875	1.20158750	1.257083200326915	7850906020.699599	99344.05903710042
	3	1.203404887789819	1.2030832	1.20308320	1.257158190890989	7870423087.973033	99470.43204300891
	4	1.205397988323746	1.2050774	1.20507740	1.257258171002197	7896442041.004807	99638.67862380833
	5	1.207892277880820	1.2075699	1.20756990	1.257383134399858	7928959622.092161	99848.58587960149
<b><math>CH</math></b>							
0	0	0.1686796335222418	0.1686344	0.16863440	1.280743635551838	146502414.5533975	13697.88432686745
1	0	0.5051421327711481	0.5050072	0.50500718	1.334184611139168	437954691.1786194	24172.55487834748
	1	0.5087256719629778	0.5085903	0.50859034	1.334753837042328	444161731.2395528	24348.44091598796
2	0	0.8416046320200543	0.841380	0.84137996	1.387625586726497	729406967.8038429	31814.20707264606
	1	0.8451881712118841	0.8449631	0.84496312	1.388194812629657	735614007.8647747	31955.83749200750
	2	0.8523507573365272	0.8521246	0.85212458	1.389332490341191	748011217.9336663	32237.18797002816
4	0	1.514529630517867	1.5141255	1.51412550	1.494507537901155	1312311521.054287	44286.10911211507
	1	1.518113169709697	1.5177087	1.51770870	1.495076763804316	1318518561.115218	44399.17187705266
	2	1.525275755834340	1.5248701	1.52487010	1.496214441515850	1330915771.184110	44624.38119780340
	3	1.536007762622479	1.5356002	1.53560020	1.497919028097772	1349469582.659151	44959.93956517626
	4	1.550295071545778	1.5498843	1.54988430	1.500188222189207	1374130067.794166	45403.23494488982
5	0	1.850992129766773	1.8504983	1.85049830	1.547948513488484	1603763797.679508	49825.13207814547
	1	1.854575668958603	1.8540815	1.85408150	1.548517739391645	1609970837.740440	49930.63590766994
	2	1.861738255083246	1.8612429	1.86124290	1.549655417103179	1622368047.809332	50140.91576569818
	3	1.872470261871385	1.8719729	1.87197290	1.551360003685101	1640921859.284373	50454.53935639852
	4	1.886757570794684	1.8862571	1.88625710	1.553629197776536	1665582344.419388	50869.41479505201
	5	1.904579645811928	1.9040761	1.90407610	1.556459955019357	1696283716.548377	51382.85392189649

Table 4: The energy eigenvalues  $E_{n,\ell}$  (in eV), the expectation values  $\langle r^2 \rangle$  (in  $(A^\circ)^2$ ),  $\langle p^2 \rangle$  (in  $(eV/c)^2$ ) and the Heisenberg Uncertainty Relations HUR (in  $eV A^\circ/c$ ) corresponding to the pseudoharmonic potential for various  $n$  and  $\ell$  quantum numbers for  $O_2$ ,  $I_2$ , LiH and HCl diatomic molecules.

$n$	$\ell$	$E_{n,\ell}$ [FM]	$\langle r^2 \rangle$	$\langle p^2 \rangle$	HUR
<i>O<sub>2</sub></i>					
0	0	6.082405894024312E-02	1.467870086578129	453449135.0159387	25799.31047672832
1	0	0.1823830803004576	1.485069856601488	1359013219.817498	44924.70998764375
	1	0.1827419925110476	1.485120537234774	1364349752.232202	45013.59613507033
2	0	0.3039421016606738	1.502269626624847	2264577304.619040	58326.71516443513
	1	0.3043010138712638	1.502320307258132	2269913837.033761	58396.38390433131
	2	0.3050169834489775	1.502421663244821	2280585790.008812	58535.47211561160
3	0	0.4255011230208900	1.519469396648205	3170141389.420599	69404.12685332494
	1	0.4258600352314801	1.519520077281491	3175477921.835303	69463.67725072471
	2	0.4265760048091938	1.519621433268180	3186149874.810354	69582.62455072057
	3	0.4276499591757634	1.519773454051252	3202155025.505520	69760.66372620103
4	0	0.5470601443811045	1.536669166671564	4075705474.222158	79139.18709888101
5	0	0.6686191657413207	1.553868936694923	4981269559.023701	87978.63395774535
<i>I<sub>2</sub></i>					
0	0	5.42449970006802E-03	7.098394036762265	320680189.5596539	47710.73616365649
1	0	1.627098533780424E-02	7.122689533744640	961765820.0079417	82766.89761060214
	1	1.628025357504326E-02	7.122710358250389	962864811.0585099	82814.29323082611
2	0	2.711747097560124E-02	7.146985030727015	1602851450.456229	107030.6279664366
	1	2.712673921284026E-02	7.147005855232764	1603950441.506798	107067.4703023858
	2	2.714527568731917E-02	7.147047504060674	1606148404.230512	107141.1169607948
3	0	3.796395661339824E-02	7.171280527709389	2243937080.904476	126853.8619581419
	1	3.797322485063725E-02	7.171301352215139	2245036071.955085	126885.1063702248
	2	3.799176132511617E-02	7.171343001043049	2247234034.678800	126947.5721166007
	3	3.801956603683410E-02	7.171405473825944	2250530930.321917	127041.2131267849
4	0	4.881044225119524E-02	7.195576024691764	2885022711.352764	144081.2279670782
5	0	5.965692788899224E-02	7.219871521674139	3526108341.801052	159555.7871069145
<i>LiH</i>					
0	0	9.710845082063990E-02	2.595085655742136	79803360.75277831	14390.84975842462
1	0	0.2908587779619696	2.693142155955575	238645395.3562673	25351.64638753563
	1	0.2927238938926831	2.694086095315485	241702867.6682745	25518.00021520058
2	0	0.4846091051032984	2.791198656169013	397487429.9597564	33308.65323527427
	1	0.4864742210340127	2.792142595528923	400544902.2717635	33442.16624345619
	2	0.4902022355989111	2.794029425531101	406653057.1155632	33707.57492853888
3	0	0.6783594322446271	2.889255156382451	556329464.5632454	40092.11610949021
	1	0.6802245481753415	2.890199095742362	559386936.8752526	40208.70078884599
	2	0.6839525627402399	2.892085925744539	565495091.7190522	40440.82585504762
	3	0.6895397804451084	2.894913554768570	574640405.9599305	40786.44750810148
4	0	0.8721097593859559	2.987311656595890	715171499.1667345	46221.64164031762
5	0	1.065860086527285	3.085368156809328	874013533.7702235	51929.31277915241
<i>HCl</i>					
0	0	0.1560617311494585	1.652050178604493	142777592.1598772	15358.24686051258
1	0	0.4675281318814175	1.706824648069883	427134412.9930121	27000.80636083549
	1	0.4701527552915152	1.707286254022739	431926335.1967491	27155.51315721777
2	0	0.7789945326133765	1.761599117535273	711491233.8261490	35402.85764796715
	1	0.7816191560234742	1.762060723488129	716283156.0298859	35526.53115822570
	2	0.7868660265436169	1.762983542268707	725858842.0084449	35772.57598316216
3	0	1.090460933345335	1.816373587000663	995848054.6592839	42530.36683534621
	1	1.093085556755433	1.816835192953519	1000639976.863021	42637.98688307097
	2	1.098332427275576	1.817758011734097	1010215662.841582	42852.39333700694
	3	1.106199168605709	1.819141258763775	1024558847.741779	43171.95005971520
4	0	1.401927334077294	1.871148056466053	1280204875.492421	48943.36384696100
5	0	1.713393734809253	1.925922525931443	1564561696.325556	54892.84665749171



Table 5: The energy eigenvalues  $E_{n,\ell}$ (in eV), the expectation values  $\langle r^2 \rangle$  (in  $(A^\circ)^2$ ),  $\langle p^2 \rangle$  (in  $(eV/c)^2$ ) and the Heisenberg Uncertainty Relations HUR (in  $eV A^\circ/c$ ) corresponding to the pseudoharmonic potential for various  $n$  and  $\ell$  quantum numbers for  $H_2$ , ScH, TiH and VH diatomic molecules.

$n$	$\ell$	$E_{n,\ell}$ [FM]	$\langle r^2 \rangle$	$\langle p^2 \rangle$	HUR
<i>H<sub>2</sub></i>					
0	0	0.3802143254317158	0.5720067969319436	179353151.5582044	10128.73248449469
1	0	1.136872065928291	0.6158608064535510	534520083.1548633	18143.59306965887
	1	1.151940622653841	0.6167341564193854	548652322.0868371	18394.90763852220
2	0	1.893529806424867	0.6597148159751585	889687014.7515233	24226.83853110614
	1	1.908598363150416	0.6605881659409929	903819253.6834971	24434.65373466418
	2	1.938664759306279	0.6623307257790985	931950074.8372046	24844.70103375790
3	0	2.650187546921444	0.7035688254967659	1244853946.348182	29594.60134800272
	1	2.665256103646993	0.7044421754626004	1258986185.280156	29780.58037104236
	2	2.695322499802856	0.7061847353007059	1287117006.433864	30148.67132212521
	3	2.740245300798563	0.7087883221856139	1328983795.005013	30691.50035878782
4	0	3.406845287418019	0.7474228350183734	1600020877.944841	34581.67348006918
5	0	4.163503027914595	0.7912768445399808	1955187809.541501	39333.12650193264
<i>ScH</i>					
0	0	7.793888021911055E-02	3.208805616306735	71740403.45470674	15172.37652846693
1	0	0.2334806033879131	3.317829166958441	214603976.5716611	26683.69038972540
	1	0.2348245288753450	3.318771086193946	217072082.5705855	26840.50206786684
2	0	0.3890223265567156	3.426852717610148	357467549.6886156	34999.83777259364
	1	0.3903662520441475	3.427794636845652	359935655.6875399	35125.28306185265
	2	0.3930526196575466	3.429677632258357	364867451.6219697	35374.81784500067
3	0	0.5445640497255191	3.535876268261853	500331122.8055699	42060.77678076121
	1	0.5459079752129510	3.536818187497358	502799228.8044953	42170.00660535145
	2	0.5485940461540562	3.538701182910063	507731024.7389241	42387.59698123697
	3	0.5526210758596637	3.541523572150610	515117708.0628493	42711.84268486642
4	0	0.7001057728943216	3.644899818913559	643194695.9225243	48418.80038470771
5	0	0.8556474960631242	3.753923369565265	786058269.0394796	54321.28962006814
<i>TiH</i>					
0	0	7.414243861897418E-02	3.229321318744519	68344509.11468062	14856.18996590873
1	0	0.2220937097705074	3.343783679169409	204419756.4028107	26144.51080359900
	1	0.2234282082928383	3.344816082070214	206873941.5371264	26305.04298826812
2	0	0.3700449809220414	3.458246039594299	340495003.6909408	34314.94569449065
	1	0.37137947494443714	3.459278442495104	342949188.8252565	34443.52966486439
	2	0.3740470655157591	3.461342241248182	347852773.6980163	34699.24349804025
3	0	0.5179962520735746	3.572708400019190	476570250.9790701	41263.13777298301
	1	0.5193307505959055	3.573740802919994	479024436.1133866	41375.22414361222
	2	0.5219983366672931	3.575804601673072	483928020.9861464	41598.46204273429
	3	0.5259964705358442	3.578897787084974	491271469.7330276	41931.01925645876
4	0	0.6659478054197630	3.687170760444080	612645498.2672009	47528.18708649129
5	0	0.8138990765712970	3.801633120868971	748720745.5553311	53351.30349471187
<i>VH</i>					
0	0	8.186329543168380E-02	3.006871384646724	75505142.31907943	15067.65581744282
1	0	0.2452318258208468	3.110465298102923	225856581.7073171	26505.07611286482
	1	0.2466633196345676	3.111373062957315	228491052.2331402	26663.10006441421
2	0	0.4086003562100107	3.214059211559122	376208021.0955538	34772.90404416337
	1	0.4100318500237314	3.214966976413514	378842491.6213778	34899.37105199667
	2	0.4128935912481992	3.216781670327672	384106583.7945811	35150.91774339026
3	0	0.5719685749984311	3.317653125015321	526559460.4837915	41796.43094308930
	1	0.5734006920136379	3.318560889869713	529193931.0096155	41906.58996631581
	2	0.5762624332381066	3.320375583783870	534458023.1828187	42126.01774122051
	3	0.5805513058658915	3.323095539010299	542342072.6561637	42452.96835630339
4	0	0.7353371053875950	3.421247038471519	676910899.8720292	48123.58477395747
5	0	0.8987056357767589	3.524840951927718	827262339.2602668	53999.70529004866

Table 6: The energy eigenvalues  $E_{n,\ell}$  (in eV), the expectation values  $\langle r^2 \rangle$  (in  $(A^o)^2$ ),  $\langle p^2 \rangle$  (in  $(eV/c)^2$ ) and the Heisenberg Uncertainty Relations HUR (in  $eV A^o/c$ ) corresponding to the pseudoharmonic potential for various  $n$  and  $\ell$  quantum numbers for CrH, MnH, CuLi and TiC diatomic molecules.

$n$	$\ell$	$E_{n,\ell}$ [FM]	$\langle r^2 \rangle$	$\langle p^2 \rangle$	HUR
<i>CrH</i>					
0	0	7.939774230820884E-02	2.923120140335614	73312725.17284806	14639.05405057451
1	0	0.2378248211383456	3.029840333495707	219259743.6216898	25774.44499377094
	1	0.2392973231890112	3.030832335554967	221972416.2499066	25937.64015425235
2	0	0.3962518999684832	3.136560526655800	365206762.0705316	33845.13427330738
	1	0.3977244020191479	3.137552528715060	367919434.6987484	33975.97022459364
	2	0.4006681974177901	3.139535505170499	373339162.6082527	34236.11479825407
3	0	0.5546789787986199	3.243280719815893	511153780.5193725	40716.27685851796
	1	0.5561514808492856	3.244272721875153	513866453.1475893	40830.41656208592
	2	0.5590952762479269	3.246255698330592	519286181.0570936	41057.71211746852
	3	0.5635070410621514	3.249227599169900	527401773.0905892	41396.23650740588
4	0	0.7131060576287567	3.350000912975986	657100798.9682143	46917.88866158374
5	0	0.8715331364588943	3.456721106136079	803047817.4170561	52686.92759785912
<i>MnH</i>					
0	0	6.791703912318869E-02	3.135496864142230	62788898.48101475	14031.19361601737
1	0	0.2034073084815335	3.260156395169919	187733167.6563940	24739.43182695390
	1	0.2047808489433400	3.261420303318240	190266106.7993997	24910.59500993260
2	0	0.3388975778398784	3.384815926197607	312677436.8317725	32532.37722563215
	1	0.3402711183016849	3.386079834345928	315210375.9747782	32669.97853786860
	2	0.3430169070893978	3.388606093133057	320270015.6021789	32943.42007620585
3	0	0.4743878471982228	3.509475457225295	437621706.0071517	39189.57306199141
	1	0.4757613876600293	3.510739365373616	440154645.1501575	39309.90001997860
	2	0.4785071764477422	3.513265624160745	445214284.7775581	39549.41266434063
	3	0.4826215955808415	3.517051128144562	452788205.0614842	39905.88011085639
4	0	0.6098781165565677	3.634134988252983	562565975.1825310	45215.49174355506
5	0	0.7453683859149125	3.758794519280671	687510244.3579102	50835.12307885000
<i>CuLi</i>					
0	0	2.088511890200140E-02	5.368123991963938	121864956.0741156	25577.06383620081
1	0	6.262381995154742E-02	5.432124528796563	365230008.4756823	44541.83300778416
	1	6.274896727143631E-02	5.432316428163798	366689388.4190958	44631.52236639918
2	0	0.1043625210010930	5.496125065629188	608595060.8772444	57835.23639534591
	1	0.1044876683209819	5.496316964996423	610054440.8206624	57905.54872077471
	2	0.1047379629607597	5.496700743029687	612972885.8630584	58045.91731707342
3	0	0.1461012220506386	5.560125602461812	851960113.2788110	68825.90528367776
	1	0.1462263693705275	5.560317501829047	853419493.2222290	68886.01704675367
	2	0.1464766640103052	5.560701279862312	856337938.2646205	69006.08284276634
	3	0.1468521059699719	5.561276895170364	860714818.9717922	69185.78926397074
4	0	0.1878399231001846	5.624126139294437	1095325165.680378	78487.24033452841
5	0	0.2295786241497302	5.688126676127061	1338690218.081940	87261.90199933894
<i>TiC</i>					
0	0	2.689705655191421E-02	3.220299274172334	240826937.3569261	27848.42565696767
1	0	8.065722427377420E-02	3.252677646120945	721873174.7872818	48456.37975504308
	1	8.079298641607657E-02	3.252759443059853	724303654.1180329	48538.49555327389
2	0	0.1344173919956333	3.285056018069556	1202919412.217638	62862.21165659258
	1	0.1345531541379357	3.285137815008464	1205349891.548389	62926.46906542558
	2	0.1348246784225422	3.285301402622239	1210210477.970561	63054.78713582985
3	0	0.1881775597174924	3.317434390018167	1683965649.648004	74742.52844098581
	1	0.1883133218597957	3.317516186957075	1686396128.978745	74797.36930874464
	2	0.1885848461444013	3.317679774570850	1691256715.400927	74906.9302408630
	3	0.1889925427288395	3.317925140333806	1698546664.649718	75070.97095862975
4	0	0.2419377274393515	3.349812761966778	2165011887.078360	85160.93264604882
5	0	0.2956978951612106	3.382191133915389	2646058124.508715	94601.66134132190

Table 7: The energy eigenvalues  $E_{n,\ell}$  (in eV), the expectation values  $\langle r^2 \rangle$  (in  $(A^o)^2$ ),  $\langle P^2 \rangle$  (in  $(eV/c)^2$ ) and the Heisenberg Uncertainty Relations HUR (in  $eVA^o/c$ ) corresponding to the pseudoharmonic potential for various  $n$  and  $\ell$  quantum numbers for NiC, ScN, ScF and  $Ar_2$  diatomic molecules.

$n$	$\ell$	$E_{n,\ell}$ [FM]	$\langle r^2 \rangle$	$\langle P^2 \rangle$	HUR
<b>NiC</b>					
0	0	2.969207342798175E-02	2.641775184923072	276052154.6005498	27004.95754057539
1	0	8.903609107369803E-02	2.670024239769140	827415521.7954127	47002.33504364418
	1	8.919546221483721E-02	2.670100162872615	830379193.4841548	47087.10672538792
2	0	0.1483801087194152	2.698273294615207	1378778888.990264	60994.44446293167
	1	0.1485394798605535	2.698349217718682	1381742560.679018	61060.82179021862
	2	0.1488586749017538	2.698501057345057	1387669390.331840	61193.36007326155
3	0	0.2077241263651315	2.726522349461275	1930142256.185127	72543.61446142835
	1	0.2078834975062698	2.726598272564750	1933105927.873869	72600.29809598284
	2	0.2082026925474700	2.726750112191124	1939032757.526702	72713.53236590972
	3	0.2086808059708858	2.726977855182097	1947921718.028147	72883.05282225095
4	0	0.2670681440108478	2.754771404307343	2481505623.379979	82679.98990635540
5	0	0.3264121616565641	2.783020459153410	3032868990.574830	91872.39221170690
<b>ScN</b>					
0	0	3.380444182356435E-02	3.137410325933636	336542668.3090815	32494.19090653237
1	0	0.1013822471073453	3.160572203976006	1009005150.475157	56471.52939544323
	1	0.1015080480754342	3.160615110101562	1011496529.811182	56541.58837472217
2	0	0.1689600523911281	3.183734082018375	1681467632.641253	73166.56210217006
	1	0.1690858533592170	3.183776988143932	1683959011.977278	73221.23975535276
	2	0.1693353929844399	3.183862798628290	1688941565.477345	73330.47265209974
3	0	0.2365378576749109	3.206895960060745	2353930114.807349	86883.88213840939
	1	0.2366636586429980	3.206938866186301	2356421494.143354	86930.43008455163
	2	0.2369131982682227	3.207024676670659	2361404047.643441	87023.45116336453
	3	0.2372895700170101	3.207153387980668	2368877365.027091	87162.79634659131
4	0	0.3041156629586919	3.230057838103114	3026392596.973445	98870.73949875825
5	0	0.3716934682424746	3.253219716145483	3698855079.139521	109695.8899440701
<b>ScF</b>					
0	0	3.373955790469907E-02	3.227717235471636	420001022.2062209	36819.07845520750
1	0	0.1011947411226970	3.246272807998829	1259398134.700247	63940.20581075619
	1	0.1012925231418258	3.246299552935829	1261817839.752488	64001.86473123229
2	0	0.1686499243406931	3.264828380526023	2098795247.194306	82778.05438613001
	1	0.1687477063598237	3.264855125463022	2101214952.246547	82826.09737601837
	2	0.1689422411136725	3.264908614670295	2106054241.710537	82922.09980893905
3	0	0.2361051075586893	3.283383953053217	2938192359.688364	98220.23032341320
	1	0.2362028895778199	3.283410697990216	2940612064.740605	98261.06610457877
	2	0.2363974243316687	3.283464187197489	2945451354.204563	98342.68674722603
	3	0.2366887118202357	3.283544419341662	2952709986.821642	98464.99072849496
4	0	0.3035602907766872	3.301939525580410	3777589472.182390	111684.2513052555
5	0	0.3710154739946834	3.320495098107603	4616986584.676449	123817.1285503210
<b><math>Ar_2</math></b>					
0	0	6.364744498285280E-03	6.413083011982251	319839318.8285583	45289.69090359750
1	0	1.909132682864900E-02	6.437443531035714	959213790.5225470	78580.43401941488
	1	1.910336674723512E-02	6.437466708774742	960430449.4184439	78630.39516767542
2	0	3.181790915901272E-02	6.461804050089178	1598588262.216536	101635.4470999948
	1	3.182994907759884E-02	6.461827227828205	1599804921.112433	101674.2986130609
	2	3.185441729924232E-02	6.461873583054483	1602238212.471537	101751.9571257981
3	0	4.454449148937645E-02	6.486164569142642	2237962733.910562	120481.5114104745
	1	4.455653140796256E-02	6.486187746881669	2239179392.806459	120514.4719139207
	2	4.458099962960604E-02	6.486234102107946	2241612684.165525	120580.3658799896
	3	4.461711938536572E-02	6.486303634317930	2245262555.124323	120679.1393377532
4	0	5.727107381974017E-02	6.510525088196106	2877337205.604551	136868.4626358041
5	0	6.999765615010389E-02	6.534885607249569	3516711677.298540	151595.8723871621

by using Hellmann-Feynman theorem, the expectation values of  $r^2$  and  $p^2$  are obtained. The Heisenberg uncertainty products  $P_{n,\ell}$  for this potential are obtained also.

The solutions obtained have been applied to compute the explicit bound state energies for some selected diatomic molecules. The selected diatomic molecules composed of the some homogeneous diatomic molecules (dimers) ( $O_2, I_2, N_2, H_2$  and  $Ar_2$ ); the heterogeneous diatomic molecules (CO, NO, HCl, CH and LiH); the neutral transition metal hydrides ( ScH, TiH, VH, CrH and MnH); the transition-metal lithide (CuLi); the transition-metal carbides (TiC and NiC); the transition-metal nitrite (ScN) and the transition-metal fluoride(ScF).

The explicit bound state energies obtained for these diatomic molecules for various values of  $n$  and  $\ell$  are compared with the exact method [34] and the Nikiforov-Uvarov method [35] for CO, NO, CH and  $N_2$  and our results are in excellent agreement with their results as displayed in Tables 2 - 7.

Though, slight differences are noticed in the explicit bound state energies we obtained when compared with the results of Ikhdair and Sever and Sever et al. [34, 35] , this is due to the conversions used by Ikhdair and Sever and Sever et al. [34, 35] as cited in the work of Ikhdair [43], they have used the following conversions:  $1\text{amu} = 931.502 \text{ MeV}/c^2$ ,  $1\text{cm}^{-1} = 1.23985 \times 10^{-4} \text{ eV}$ , and  $\hbar c = 1973.29 \text{ eV } \text{\AA}$  (cf. pp. 791, Bransden and Joachain (2000) [75]). In our calculations, we have used the following recent conversions:  $1\text{amu} = 931.494\,028 \text{ MeV}/c^2$ ,  $1\text{cm}^{-1} = 1.239841875 \times 10^{-4} \text{ eV}$ , and  $\hbar c = 1973.29 \text{ eV } \text{\AA}$  (cf. pp. 4, Nakamura et al. (2010) in the 2010 edition of the Review of Particle Physics[76]). This explains the reason for the slight differences.

In addition, we obtained the numerical values of the expectation values of  $r^2$  and  $p^2$ , and the Heisenberg uncertainty product for these diatomic molecules. These results are displayed together with the explicit bound state energies of these diatomic molecules for various values of  $n$  and  $\ell$  in Tables 2 - 7. The Heisenberg uncertainty products obtained are valid in each case of these diatomic molecules for various  $n$  and  $\ell$ , as expected from equation (49) that

$$P_{n,\ell} \geq 2959.89 \text{ eV } \text{\AA}^o/c. \quad (51)$$

This implies that the numerical value of the Heisenberg uncertainty product  $P_{n,\ell}$

can not be less than  $2959.89 \text{ eVA}^o/c$  for this principle to hold. The Heisenberg uncertainty products in all these selected diatomic molecules attains its minimum value of  $2959.89 \text{ eVA}^o/c$ , even the lowest Heisenberg uncertainty products (for ground state)  $P_{0,0}$  obtained for  $H_2$  is  $10128.73248449469 \text{ eVA}^o/c$  which is greater than the minimum.

It is evident from the Tables displayed that the explicit bound state energies, the expectation values of  $r^2$  and  $p^2$  and the Heisenberg uncertainty products  $P_{n,\ell}$  increase as the quantum numbers  $(n, \ell)$  of the state increase. Similar studies involving the confined diatomic molecules are currently in progress [77].

It should be noted that the advantage of this SGA method is that, it allows one to find the explicit bound state energies and the eigenfunctions directly in a simple and unique way. This method, as applied here to the diatomic molecules demonstrates that the values obtained are in excellent agreement with earlier results derived from the other methods. We have also demonstrated that the Heisenberg uncertainty product is validated by all the diatoms considered. Finally, the method serves as a very useful link for finding the matrix elements from the creation and annihilation operators in addition to allowing the construction of the coherent states.

[Note to the desk Editor: Please, put the figure in the section 2, where it is indicated in the text]

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